Supplementary material

Roeperone A, a new tetraoxygenated xanthone and other compounds from the leaves of *Hypericum roeperianum* Schimp. (Hypericaceae).

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ABSTRACT

Chemical investigation of the methanol extract from the leaves of *H. roeperianum* led to the isolation of a new tetraoxygenated xanthone along with eleven known compounds including six xanthones, one polyketide, one flavonoid, one ferulic acid derivative and two pentacyclic triterpenoids. Their structures were established on the basis of 1D- and 2D-NMR, UV, IR, and MS experiments, and by comparison of their spectroscopic data with those of similar compounds reported in the literature. The new xanthone was tested against a panel of eight bacterial strains including six Gram-negative and two Gram-positive bacteria. As results, it exhibited weak antibacterial activity with MIC values ranging from 64 to 128 µg/mL.

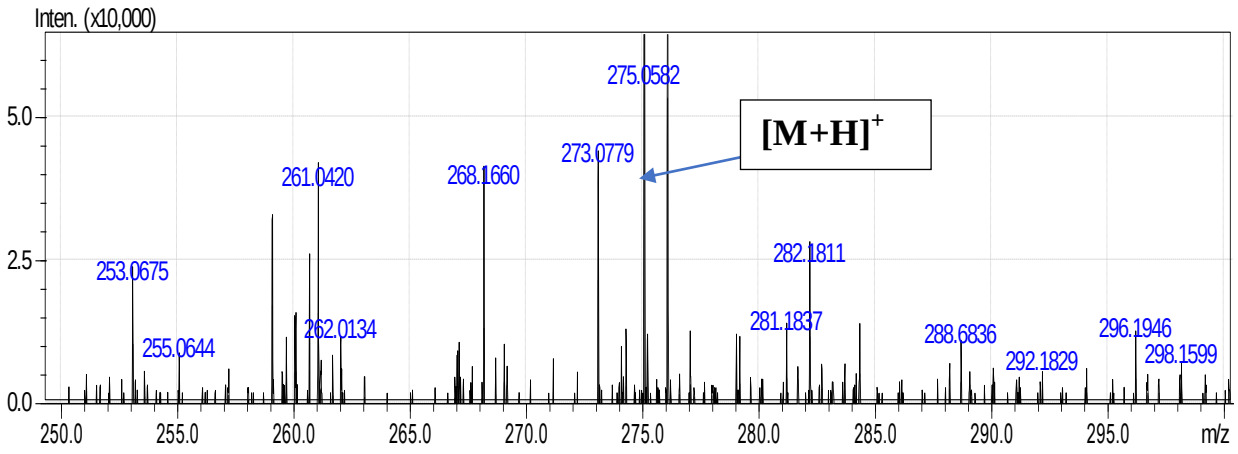


Figure 1S: (+) – HRESIMS spectrum of **1**

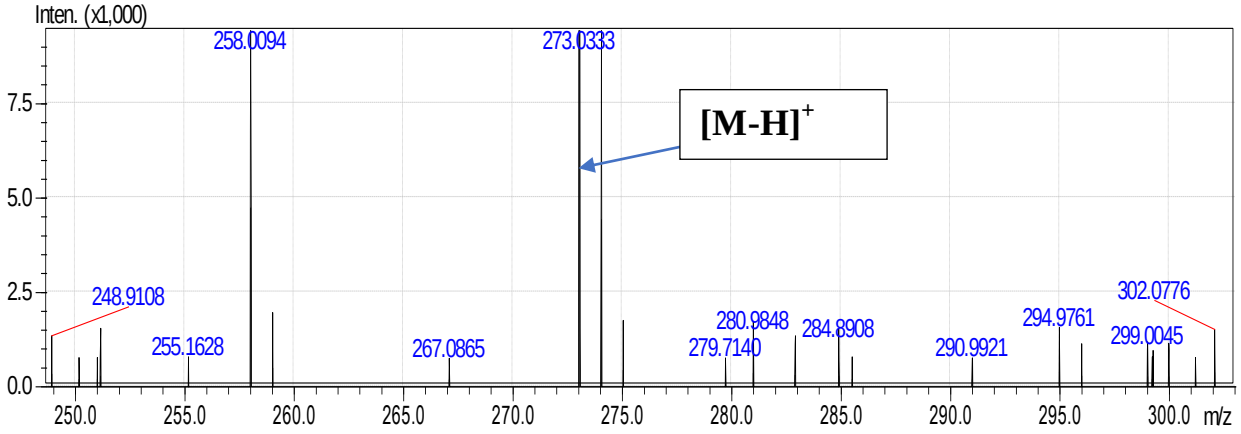


Figure 2S: (–) – HRESIMS spectrum of **1**

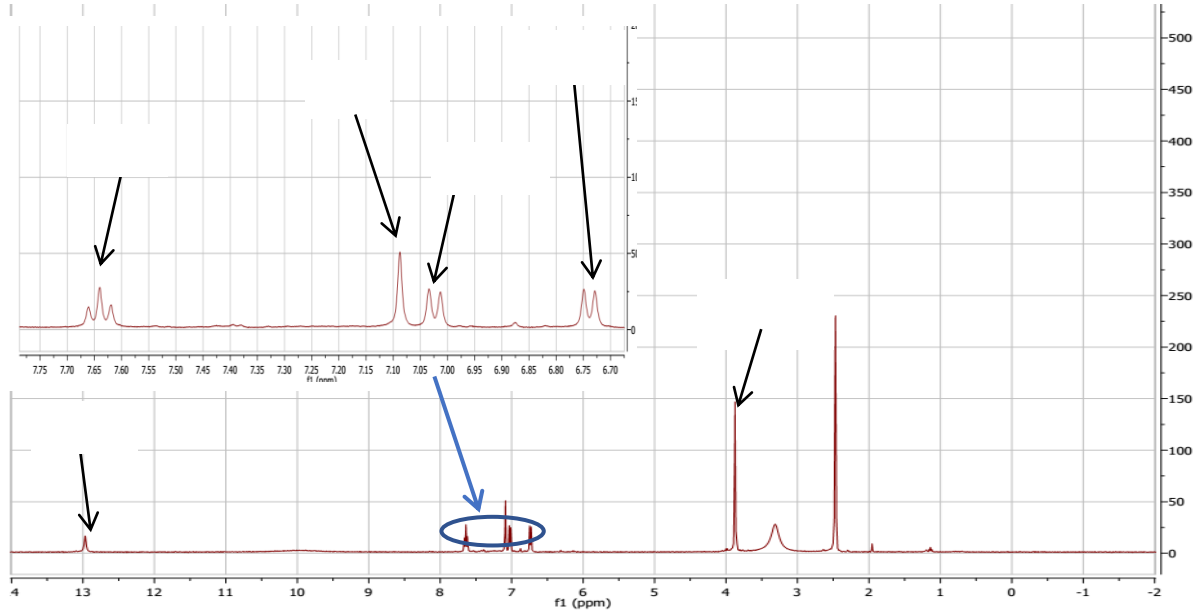


Figure 3S: ^{1}H NMR (400 MHz, DMSO-d_6) spectrum of **1**

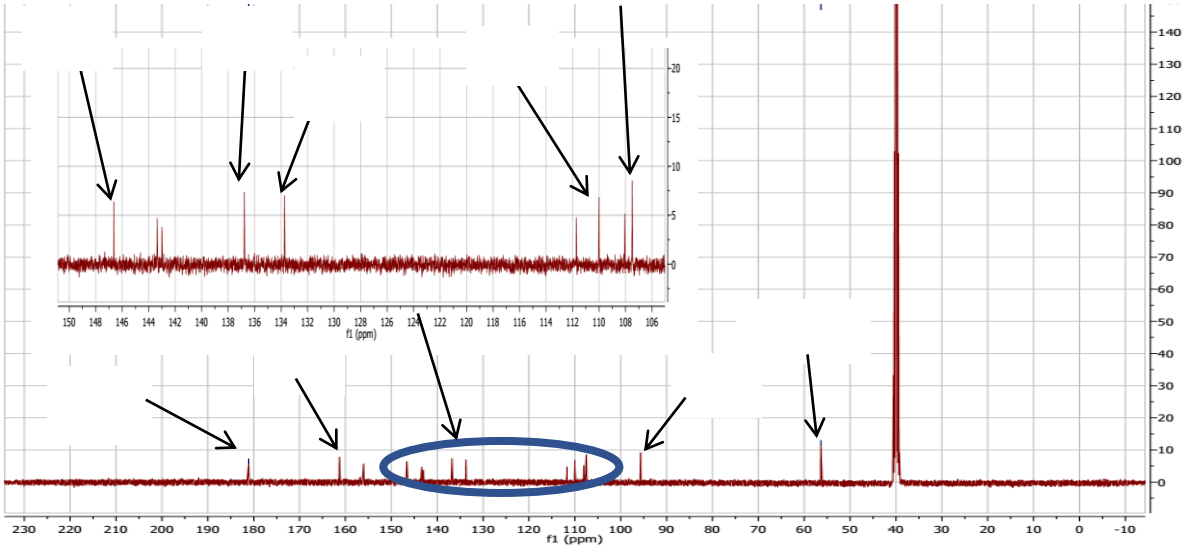


Figure 4S: ^{13}C NMR (100 MHz, DMSO-d_6) spectrum of **1**

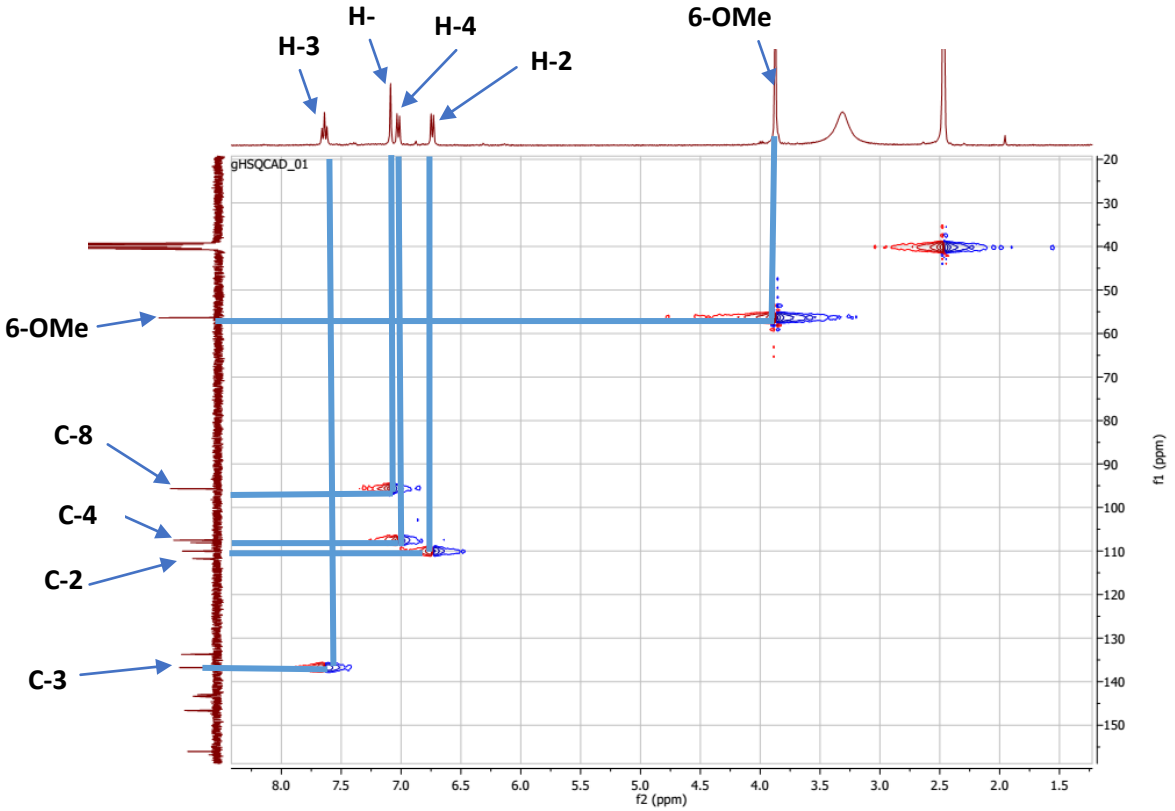


Figure 5S: HMQC (400 MHz, DMSO-d_6) spectrum of **1**

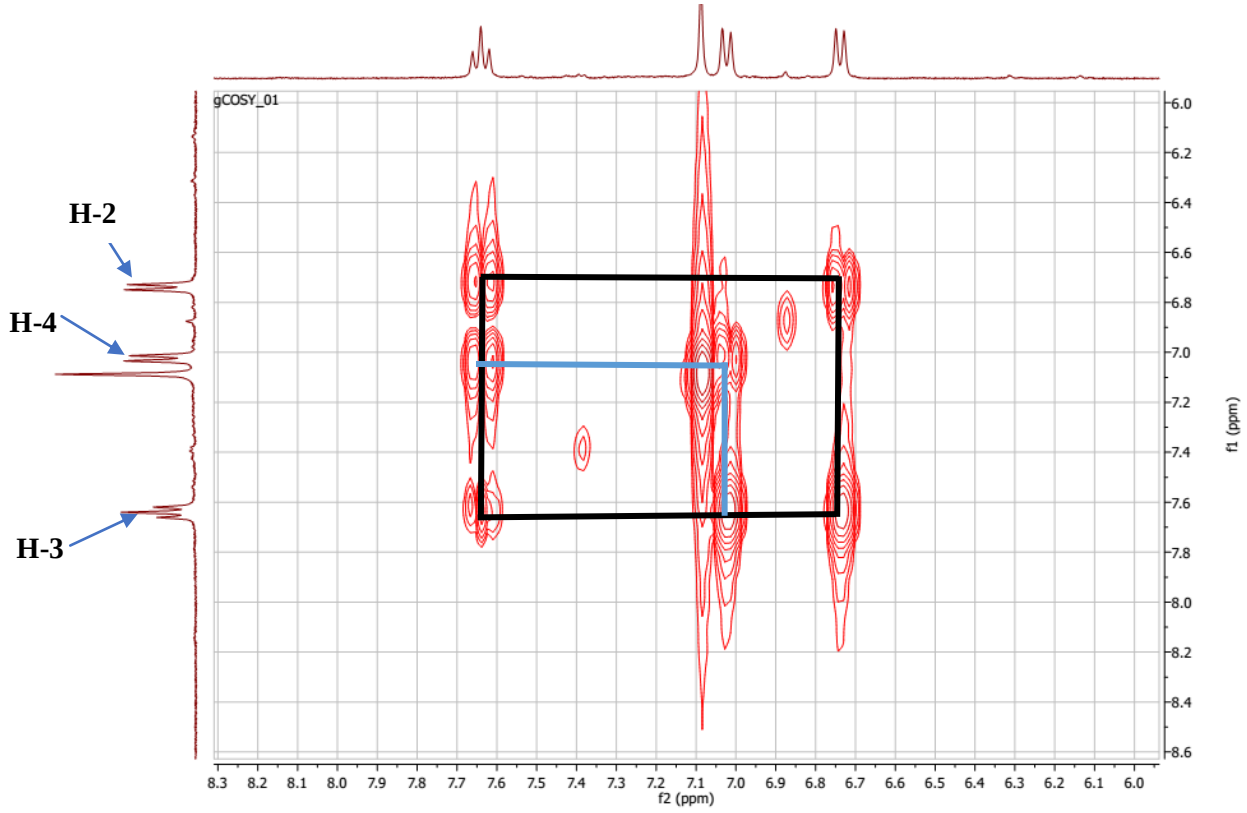


Figure 6S: ^{1}H-^{1}H COSY (400 MHz, DMSO-d_6) spectrum of **1**

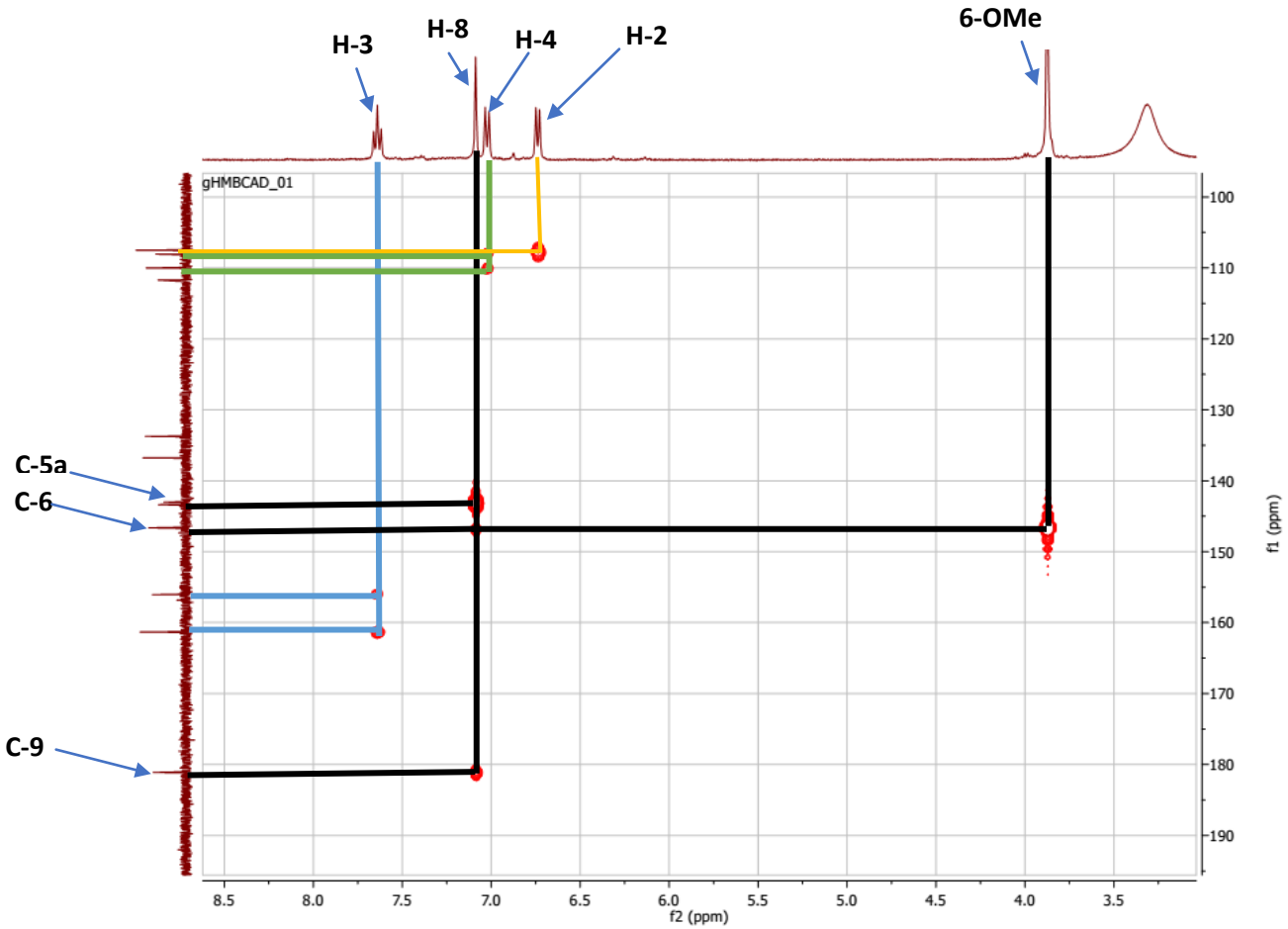


Figure 7S: HMBC (400 MHz, DMSO-d_6) spectrum of **1**

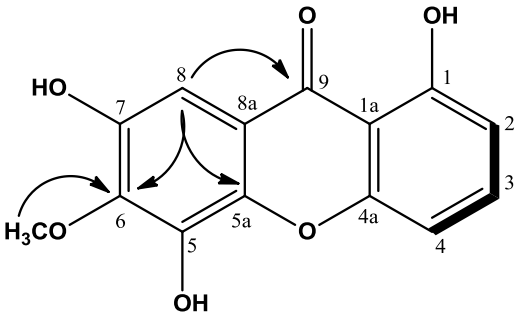


Figure 2: Key HMBC (H → C) and ^{1}H–^{1}H COSY (▬) correlations of **1**

Table 1. Antibacterial activity of Roeperone A (**1**)

Bacterial strains		**1**		CHL	
		MIC **(μg/mL)**	MBC **(μg/mL)**	MIC **(μg/mL)**	MBC **(μg/mL)**
Escherichia coli	ATCC8739	64	-	8	64
	AG102	128	-	4	16
Klebsiella pneumoniae	ATCC11296	64	64	2	64
	KP55	64	-	2	16
Providencia stuartii	ATCC29916	128	-	16	64
	PS2636	128	-	64	256
Staphylococcus aureus	ATCC25923	-	-	16	256
	MRSA3	128	-	32	256

- : ≥ 128 μg/mL; MIC: minimum inhibitory concentration; MBC: minimum bactericidal concentration; CHL: Chloramphenicol.

NMR data of known compounds

1,5-dihydroxy-8-methoxyxanthone **(2)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 161.6 (C-1), 111.4 (C-1a), 137.2 (C-2), 107.0 (C-3), 152.6 (C-4), 146.2 (C-4a), 139.6 (C-5), 122.2 (C-5a), 106.4 (C-6), 155.2 (C-7), 109.1 (C-8), 110.6 (C-8a), 182.5 (C-9), 56.6 (8-OCH_3); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.72 (1H, d, 8.4, H-2), 7.63 (1H, t, 8.4, H-3), 6.97 (1H, d, 8.4, H-4), 7.28 (1H, d, 9.2, H-6), 6.81 (1H, d, 9.2, H-7), 3.80 (3H, s, 8-OCH_3), 13.07 (1H, s, 1-OH), 9.78 (3H, brs, 5-OH).

1,3,5,7-tetrahydroxyxanthone **(3)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 165.1 (C-1), 102.0 (C-1a), 94.0 (C-2), 163.0 (C-3), 98.1 (C-4), 157.7 (C-4a), 154.6 (C-5), 151.3 (C-5a), 103.0 (C-6), 144.2 (C-7), 108.3 (C-8), 112.1 (C-8a), 179.3 (C-9); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.29 (1H, d, 1.0, H-2), 6.11 (1H, d,

1.0, H-4), 6.82 (1H, d, 1.0, H-6), 7.33 (1H, d, 1.0, H-8), 13.1 (1H, s, 1-OH), 10.4 (3H, s, 3,5,7-OH).

1,3,5,6-tetrahydroxyxanthone **(4)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 163.3 (C-1), 101.8 (C-1a), 98.2 (C-2), 165.5 (C-3), 94.3 (C-4), 157.7 (C-4a), 132.9 (C-5), 146.4 (C-5a), 152.3 (C-6), 113.4 (C-7), 116.2 (C-8), 116.3 (C-8a), 180.1 (C-9); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.13 (1H, d, 1.6, H-2), 6.37 (1H, d, 1.6, H-4), 6.89 (1H, d, 8.4, H-7), 7.47 (1H, d, 8.4, H-8), 13.10 (1H, brs, 1-OH).

5-hydroxy-1,3-dimethoxyxanthone **(5)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 161.9 (C-1), 106.7 (C-1a), 95.7 (C-2), 165.1 (C-3), 93.5 (C-4), 159.3 (C-4a), 146.4 (C-5), 144.2 (C-5a), 124.1 (C-6), 119.5 (C-7), 115.5 (C-8), 115.3 (C-8a), 174.2 (C-9), 56.4 (1-OCH_3), 56.6 (3-OCH_3); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.47 (1H, d, 2.0, H-2), 6.65 (1H, d, 2.0, H-4), 7.15 (1H, d, 7.6, H-6), 7.17 (1H, t, 7.6, H-7), 7.45 (1H, d, 7.6, H-8), 3.84 (3H, s, 3-OCH_3), 4.88 (3H, s, 5-OCH_3), 10.3 (1H, s, 5-OH).

2-hydroxy-5-methoxyxanthone **(6)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 106.0 (C-1), 121.7 (C-1a), 156.1 (C-2), 125.2 (C-3), 120.4 (C-4), 150.6 (C-4a), 147.1 (C-5), 145.6 (C-5a), 120.3 (C-6), 124.4 (C-7), 115.6 (C-8), 122.1 (C-8a), 176.4 (C-9), 56.2 (5-OMe); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 7.56 (1H, d, 2.0, H-1), 7.50 (1H, dd, 6.0; 2,0, H-3), 7.66 (1H, d, 6.0, H-4), 7.32 (1H, dd, 5.2; 2.0, H-6), 7.26 (1H, t, 5.0, H-7), 7.62 (1H, dd, 5.2, 2.0, H-8), 3.89 (3H, s, 5-OMe), 9.99 (1H, brs, 2-OH).

Hyperielliptone D **(7)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 97.7 (C-1), 115.2 (C-1a), 147.1 (C-2), 140.9 (C-3), 133.8 (C-4), 142.5 (C-4a), 119.4 (C-5), 136.1 (C-6), 156.6 (C-5a), 125.6 (C-7), 127.2 (C-8), 122.0 (C-8a), 176.0 (C-9), 126.8 (C-1') 106.9 (C-2'), 149.2 (C-3'), 137.5 (C-4'), 149.2 (C-5'), 106.9 (C-6'), 78.0 (C-7'), 79.0 (C-8'), 61.1 (C-9'), 57.4 (3',5'-OMe), 57.0 (2-OMe); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 7.18 (1H, s, H-1), 7.66 (1H, d, 5.6, H-5), 7.82 (1H, t, 6.0, H-6), 7.45

(1H, t, 6.0, H-7), 8.18 (1H, d, 5.6, H-8), 6.75 (1H, s, H-2'), 6.75 (1H, s, H-6'), 5.08 (1H, m, H-7'), 4.42 (1H, m, H-8'), 3.68 (1H, m, H-9'a), 3.42 (1H, m, H-9'b), 3.74 (6H, s, 3',5'-OMe), 3.84 (3H, s, 2-OMe).

4-methoxy-3-(2-methylbut-3-en-2-yl)-6-phenyl-2H-pyran-2-one **(8)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 163.9 (C-2), 110.5 (C-3), 168.4 (C-4), 93.6 (C-5), 159.3 (C-6), 131.0 (C-1'), 125.3 (C-2'), 128.7 (C-3'), 130.7 (C-4'), 128.7 (C-5'), 125.3 (C-6'), 39.5 (C-1"), 148.3 (C-2"), 107.2 (C-3"), 26.9 (C-4"), 26.9 (C-5"), 55.6 (4-OCH_3); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.88 (1H, s, H-5), 7.81 (2H, m, H-2',6'), 7.39 (2H, m, H-3',5'), 7.41 (1H, m, H-4'), 6.05 (1H, dd, 8.5, 15.5, H-2"), 4.82 (1H, d, 15.2, H-3"a), 4.74 (1H, d, 8.5, H-3"b), 1.39 (3H, s**,** H-4"), 1.39 (3H, s**,** H-5"), 3.86 (3H, s**,** 4-OCH_3).

8,8-bis-(dihydroconiferyl)-diferulate **(9)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 131.2 (C-1), 113.1 (C-2), 147.8 (C-3), 145.1 (C-4), 114.8 (C-5), 121.4 (C-6), 34.2 (C-7), 37.2 (C-8), 64.2 (C-9), 126.0 (C-1'), 111.5 (C-2'), 148.4 (C-3'), 149.8 (C-4'), 115.9 (C-5'), 123.7 (C-6'), 145.6 (C-7'), 115.8 (C-8'), 167.2 (C-9'), 56.1 (3-OMe), 55.7 (3'-OMe); ^{1} H NMR (400 MHz, DMSO-d_6): δ_H 6.67 (1H, s, H-2), 6.66 (1H, d, 6.5, H-5), 6.54 (1H, d, 6.5, H-6), 2.58 (1H, dd, 8.8, 4.0, H-7a), 2.74 (1H, dd, 8.8, 4.0, H-7b), 2.19 (1H, m, H-8), 4.08 (1H, dd, 7.6, 3.6, H-9a), 4.28 (1H, dd, 7.6, 3.6, H-9b), 7.30 (1H, s, H-2'), 6.78 (1H, d, 7.0, H-5'), 7.10 (1H, d, 7.0, H-6'), 7.53 (1H, d, 13.5, H-7'), 6.59 (1H, d, 13.5, H-8'), 3.67 (3H, s, 3-OCH_3), 3.81 (3H, s, 3'-OCH_3), 8.75 (1H, s, 4-OH), 9.64 (1H, s, 4'-OH).

Friedelin **(10)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 22.3 (C-1), 41.6 (C-2), 213.2 (C-3), 58.3 (C-4), 42.2 (C-5), 41.3 (C-6), 18.3 (C-7), 53.1 (C-8), 37.5 (C-9), 59.5 (C-10), 35.7 (C-11), 30.5 (C-12), 39.3 (C-13), 38.3 (C-14), 32.5 (C-15), 36.1 (C-16), 30.0 (C-17), 42.8 (C-18), 35.4 (C-19), 28.2 (C-

20), 32.8 (C-21), 39.7 (C-22), 6.8 (C-23), 14.7 (C-24), 18.0 (C-25), 20.3 (C-26), 18.7 (C-27), 32.1 (C-28), 35.1 (C-29), 31.8 (C-30).

Trichadonic acid **(11)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 22.0 (C-1), 41.1 (C-2), 212.1 (C-3), 57.3 (C-4), 41.8 (C-5), 41.0 (C-6), 18.5 (C-7), 53.1 (C-8), 38.1 (C-9), 59.0 (C-10), 37.8 (C-11), 27.7 (C-12), 38.9 (C-13), 32.9 (C-14), 35.8 (C-15), 36.1 (C-16), 30.8 (C-17), 42.7 (C-18), 35.8 (C-19), 28.5 (C-20), 32.9 (C-21), 37.4 (C-22), 7.2 (C-23), 14.7 (C-24), 18.4 (C-25), 22.9 (C-26), 178.0 (C-27), 31.3 (C-28), 30.6 (C-29), 35.8 (C-30).

Quercetin **(12)**

^{13}C NMR (100 MHz, DMSO-d_6): δ_C 147.3 (C-2), 136.2 (C-3), 176.5 (C-4), 103.5 (C-4a), 161.3 (C-5), 98.7 (C-6), 164.6 (C-7), 93.7 (C-8), 156.7 (C-8a), 122.4 (C-1'), 115.5 (C-2'), 145.7 (C-3'), 148.3 (C-4'), 116.0 (C-5'), 120.4 (C-6'); ^{1}H NMR (400 MHz, DMSO-d_6): δ_H 6.20 (1H, d, 2.0, H-6), 6.41 (1H, d, 2.0, H-8), 7.76 (1H, d, 2.0, H-2'); 6.91 (1H, d, 6.8, H-5'), 7.66 (1H, dd, 6.8, 2.0, H-6').